

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric Result

logP (XH +) 0.45 ±0.04 (n=50)
 logP (neutral X) 4.08 ±0.01 (n=50)

18C-03011 Points 1 to 20

M02_octanol concentration factor 0.967
 Carbonate 0.1632 mM
 Acidity error -1.49856 mM

18C-03011 Points 21 to 48

M02_octanol concentration factor 1.157
 Carbonate 0.1227 mM
 Acidity error -1.56956 mM

18C-03011 Points 49 to 70

M02_octanol concentration factor 1.597
 Carbonate 0.1477 mM
 Acidity error -1.25180 mM

Warnings and errors

Errors None
 Warnings None

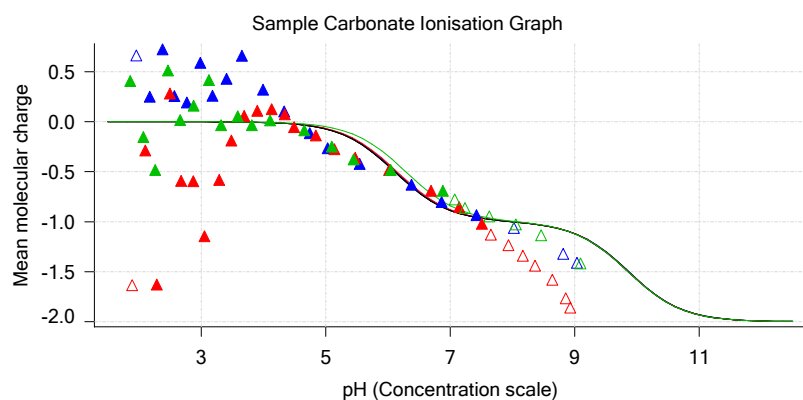
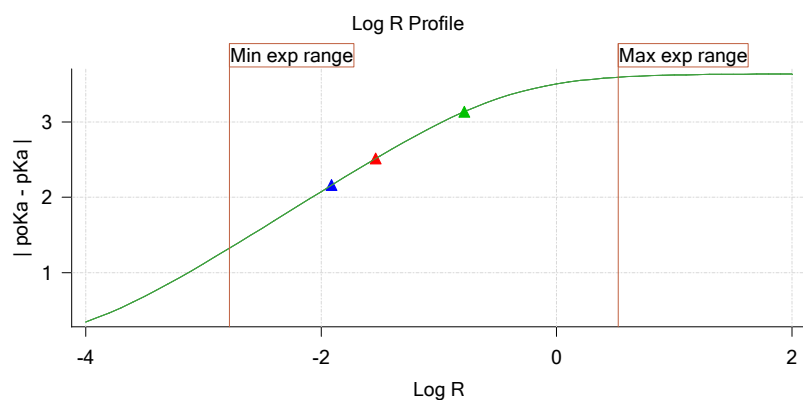
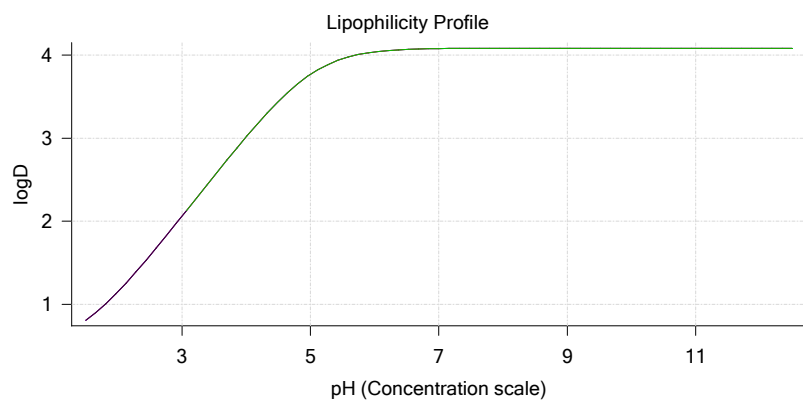
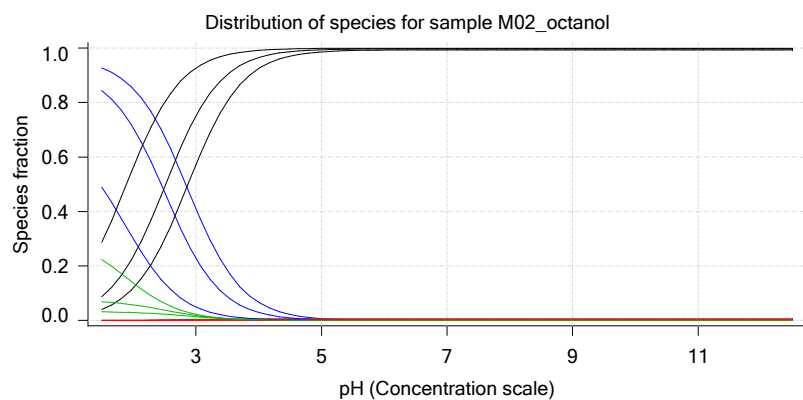
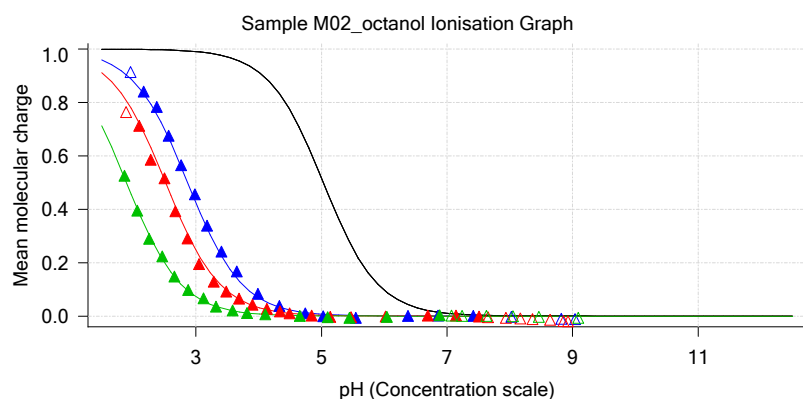
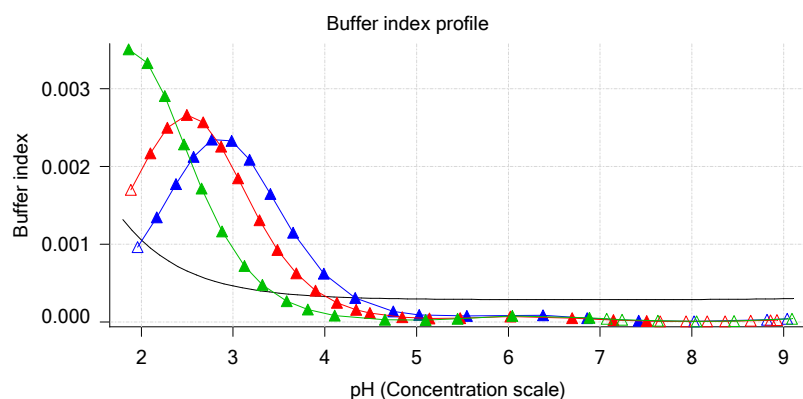
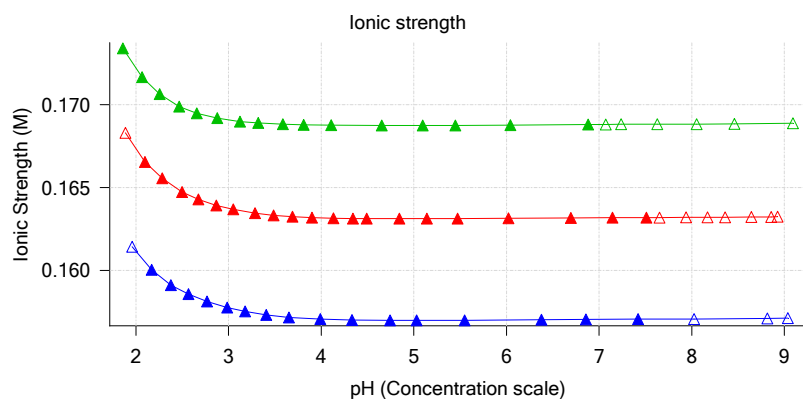
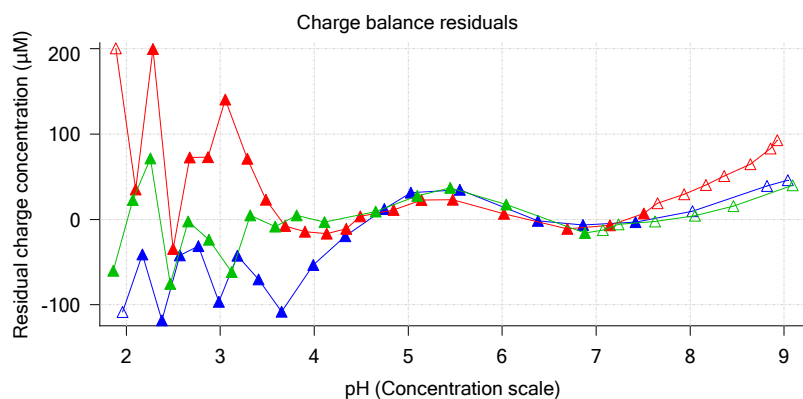
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	0.59	20.31 %	0.00 %	56.73 %	22.95 %	Stomach pH
1.200	0.66	17.91 %	0.00 %	50.02 %	32.07 %	
2.000	1.15	6.63 %	0.01 %	18.50 %	74.87 %	
3.000	2.06	0.86 %	0.01 %	2.39 %	96.74 %	
4.000	3.02	0.09 %	0.01 %	0.25 %	99.66 %	
5.000	3.77	0.01 %	0.01 %	0.02 %	99.96 %	Blood pH
6.000	4.04	0.00 %	0.01 %	0.00 %	99.99 %	
6.500	4.07	0.00 %	0.01 %	0.00 %	99.99 %	
7.000	4.08	0.00 %	0.01 %	0.00 %	99.99 %	
7.400	4.08	0.00 %	0.01 %	0.00 %	99.99 %	
8.000	4.08	0.00 %	0.01 %	0.00 %	99.99 %	
9.000	4.08	0.00 %	0.01 %	0.00 %	99.99 %	
10.000	4.08	0.00 %	0.01 %	0.00 %	99.99 %	
11.000	4.08	0.00 %	0.01 %	0.00 %	99.99 %	
12.000	4.08	0.00 %	0.01 %	0.00 %	99.99 %	

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

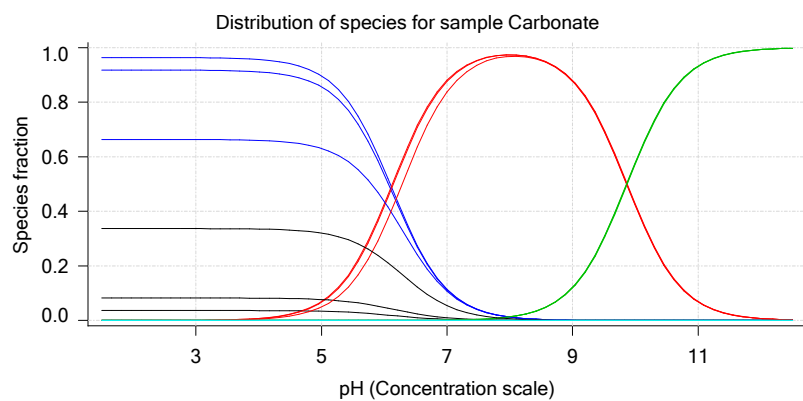
Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Graphs



Sample name:	M02_octanol	Experiment start time:	3/3/2018 1:46:01 PM
Assay name:	pH-metric high logP	Analyst:	Dorothy Levorse
Assay ID:	18C-03011	Instrument ID:	T312060
Filename:	C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r		

Graphs (continued)



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-03011 Points 1 to 20

Overall results

RMSD 0.135
 Average ionic strength 0.157 M
 Average temperature 24.9°C
 Partition ratio 0.0123 : 1
 Analyte concentration range 4180.2 µM to 4304.6 µM
 Total points considered 16 of 20

Warnings and errors

Errors None
 Warnings Excessive acidity error present

Four-Plus parameters

Alpha 0.111 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r

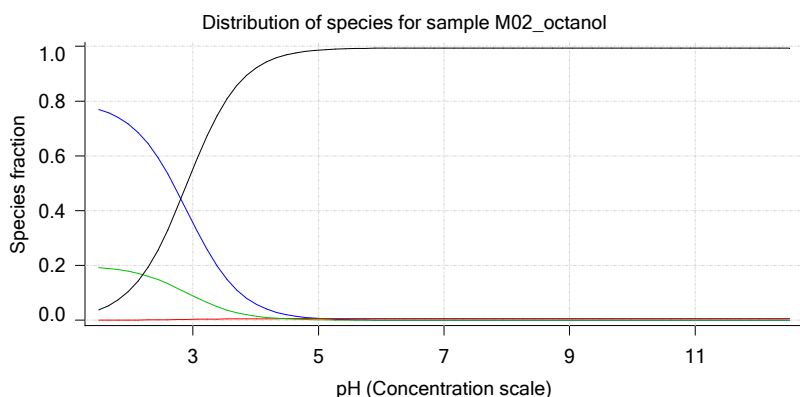
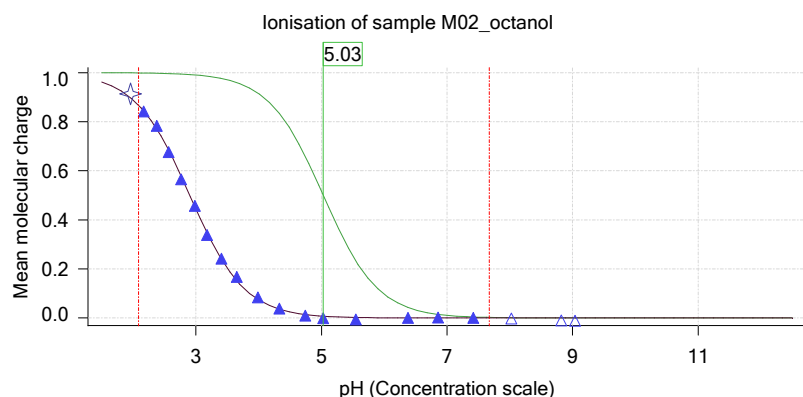
Titrants

0.50 M HCl 0.999058 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 1:46:01 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M02_octanol concentration factor 0.967
 Base pKa 1 5.03
 logP (XH +) 1.31
 logP (neutral X) 4.13

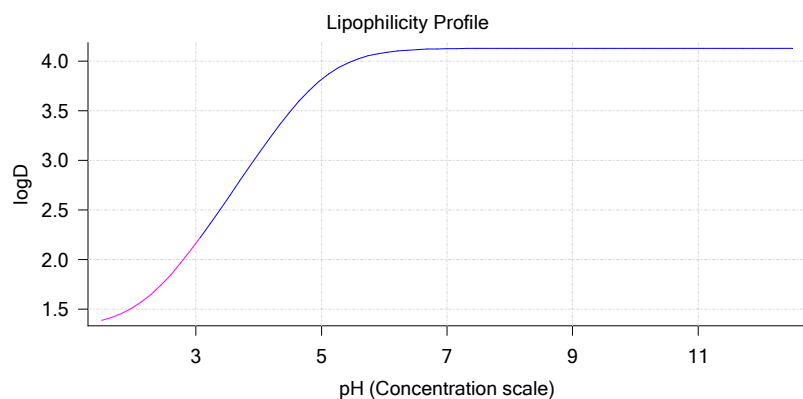
Sample graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Sample graphs (continued)



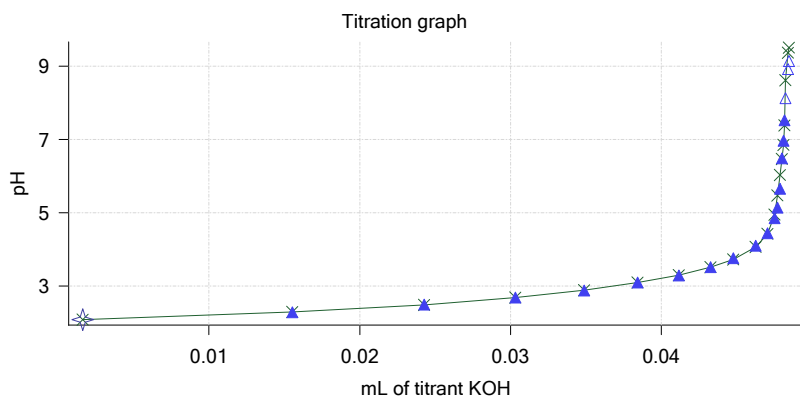
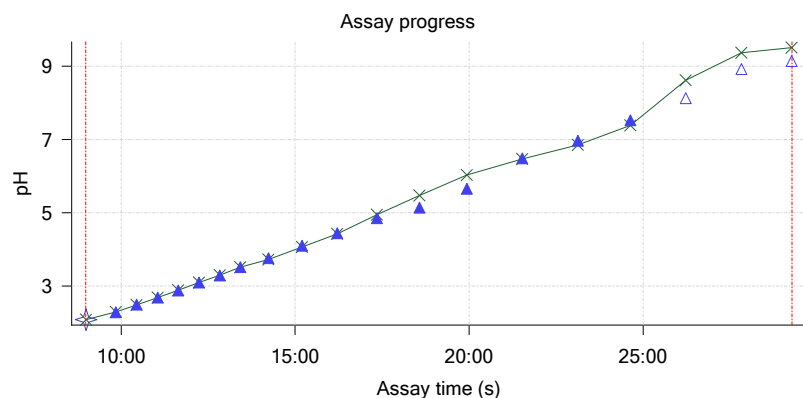
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanolH	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.33	79.02 %	0.01 %	19.74 %	1.22 %	
1.200	1.35	78.46 %	0.01 %	19.60 %	1.93 %	
2.000	1.52	71.14 %	0.07 %	17.77 %	11.02 %	
3.000	2.16	35.60 %	0.33 %	8.90 %	55.17 %	
4.000	3.07	5.94 %	0.55 %	1.48 %	92.02 %	
5.000	3.82	0.64 %	0.59 %	0.16 %	98.61 %	
6.000	4.09	0.06 %	0.60 %	0.02 %	99.32 %	
6.500	4.12	0.02 %	0.60 %	0.01 %	99.38 %	
7.000	4.13	0.01 %	0.60 %	0.00 %	99.39 %	
7.400	4.13	0.00 %	0.60 %	0.00 %	99.40 %	
8.000	4.13	0.00 %	0.60 %	0.00 %	99.40 %	
9.000	4.13	0.00 %	0.60 %	0.00 %	99.40 %	
10.000	4.13	0.00 %	0.60 %	0.00 %	99.40 %	
11.000	4.13	0.00 %	0.60 %	0.00 %	99.40 %	
12.000	4.13	0.00 %	0.60 %	0.00 %	99.40 %	

Carbonate and acidity

Carbonate 0.163 mM
 Acidity error -1.499 mM

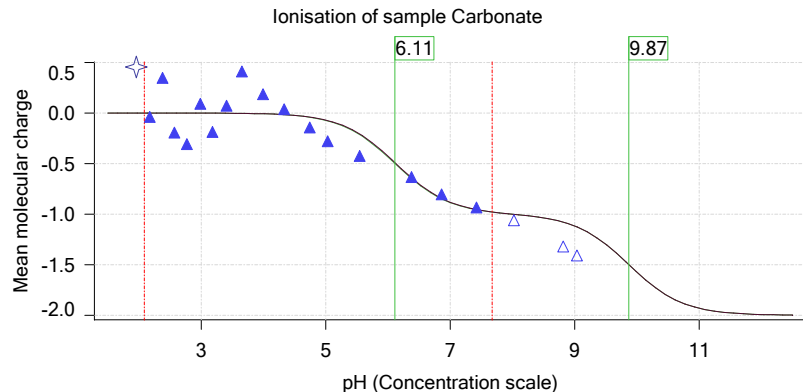
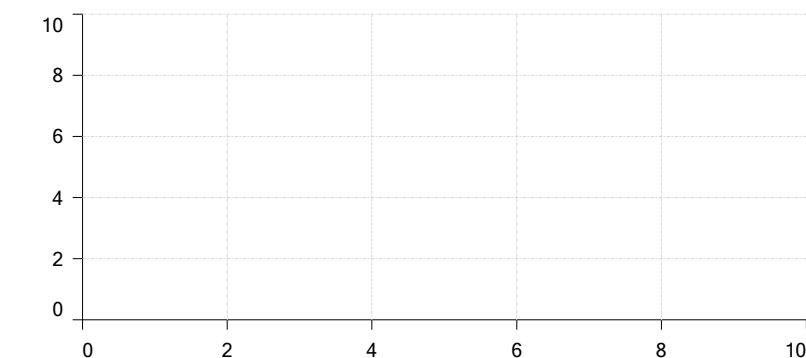
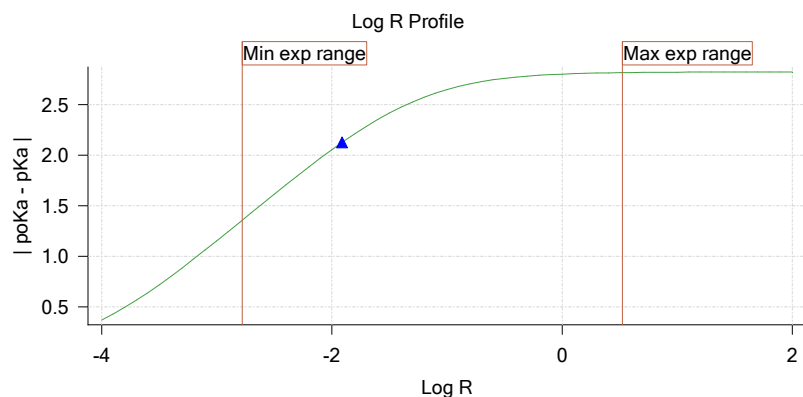
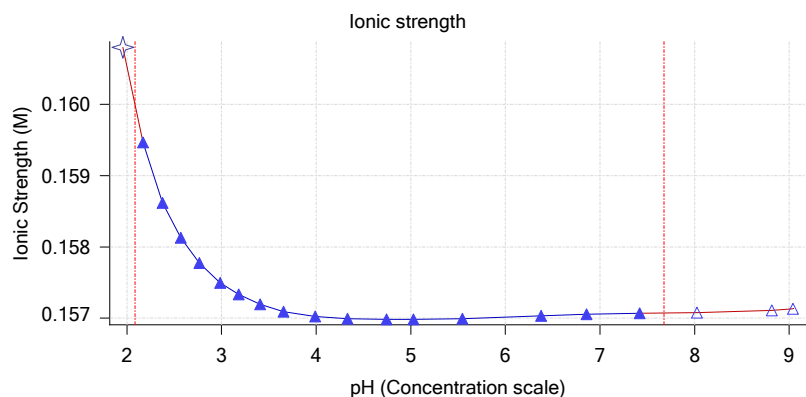
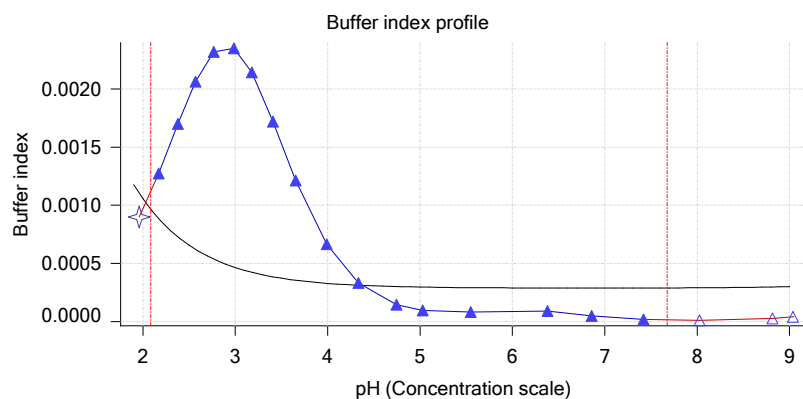
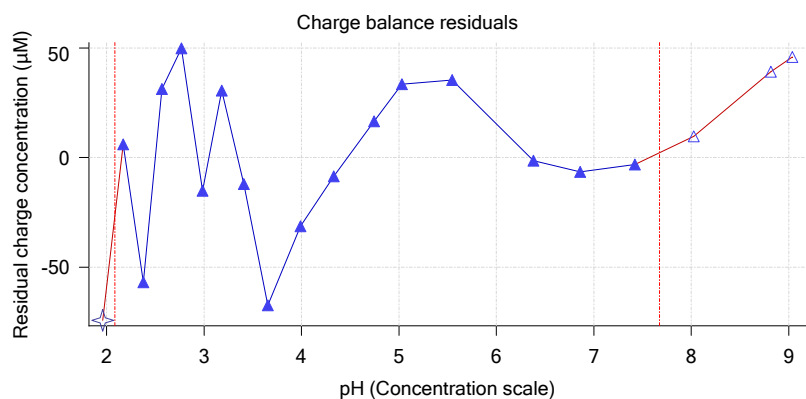
Other graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-03011 Points 21 to 48

Overall results

RMSD 0.183
 Average ionic strength 0.163 M
 Average temperature 25.0°C
 Partition ratio 0.0290 : 1
 Analyte concentration range 3843.8 µM to 3969.0 µM
 Total points considered 20 of 28

Warnings and errors

Errors None
 Warnings Excessive acidity error present

Four-Plus parameters

Alpha 0.111 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r

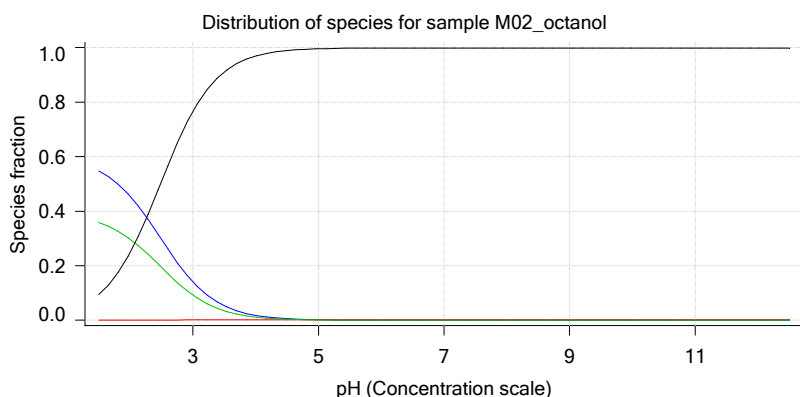
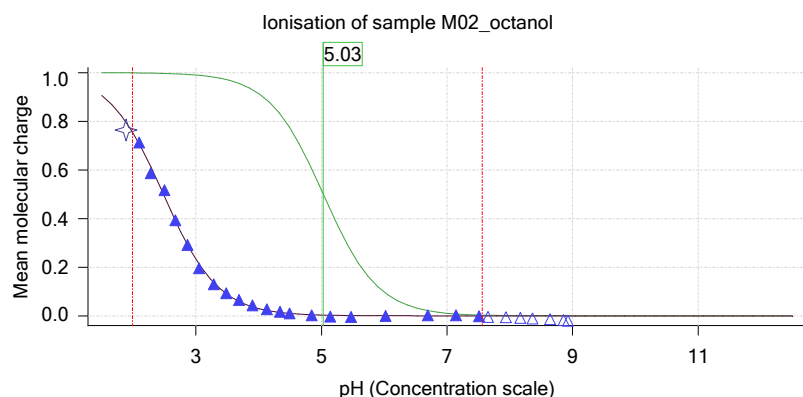
Titrants

0.50 M HCl 0.999058 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 1:46:01 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M02_octanol concentration factor 1.157
 Base pKa 1 5.03
 logP (XH +) 1.35
 logP (neutral X) 4.30

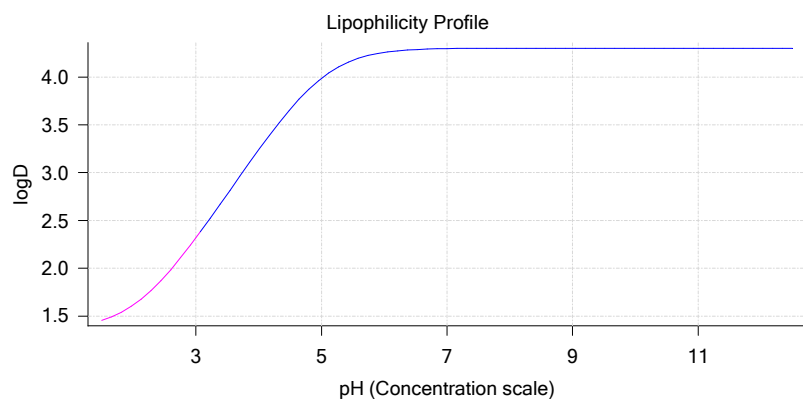
Sample graphs



Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03011**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Sample graphs (continued)



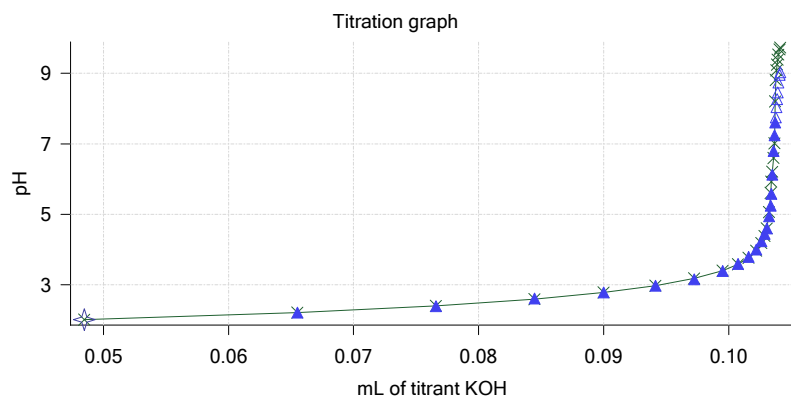
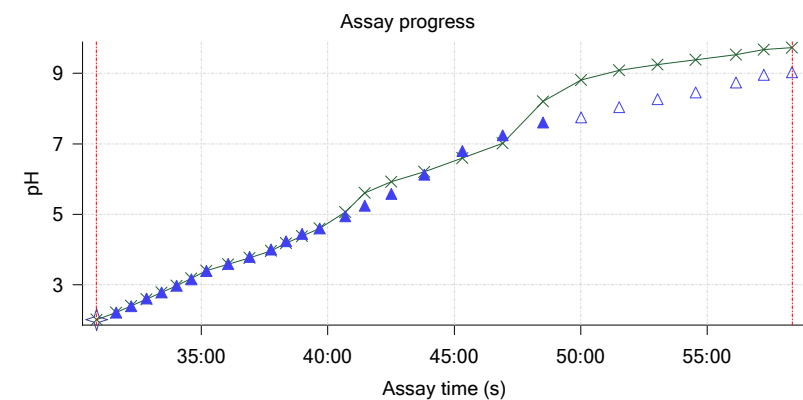
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.39	58.55 %	0.01 %	38.26 %	3.18 %	Stomach pH
1.200	1.41	57.48 %	0.01 %	37.56 %	4.95 %	
2.000	1.61	45.50 %	0.04 %	29.73 %	24.72 %	
3.000	2.32	14.10 %	0.13 %	9.21 %	76.56 %	
4.000	3.24	1.78 %	0.17 %	1.17 %	96.88 %	
5.000	3.99	0.18 %	0.17 %	0.12 %	99.53 %	Blood pH
6.000	4.26	0.02 %	0.17 %	0.01 %	99.80 %	
6.500	4.29	0.01 %	0.17 %	0.00 %	99.82 %	
7.000	4.30	0.00 %	0.17 %	0.00 %	99.83 %	
7.400	4.30	0.00 %	0.17 %	0.00 %	99.83 %	
8.000	4.30	0.00 %	0.17 %	0.00 %	99.83 %	
9.000	4.30	0.00 %	0.17 %	0.00 %	99.83 %	
10.000	4.30	0.00 %	0.17 %	0.00 %	99.83 %	
11.000	4.30	0.00 %	0.17 %	0.00 %	99.83 %	
12.000	4.30	0.00 %	0.17 %	0.00 %	99.83 %	

Carbonate and acidity

Carbonate 0.123 mM
Acidity error -1.570 mM

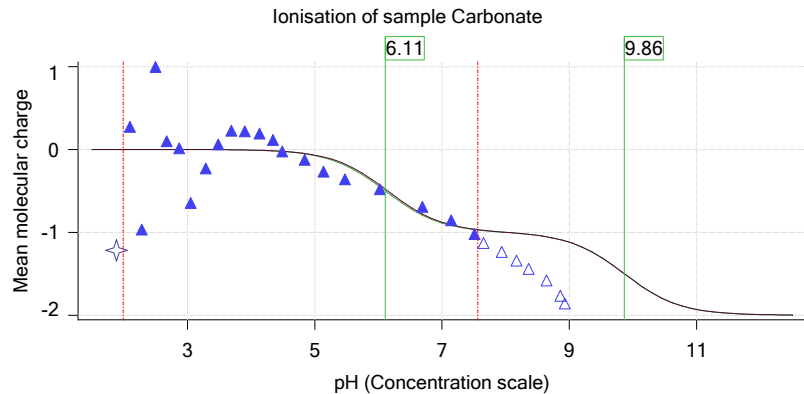
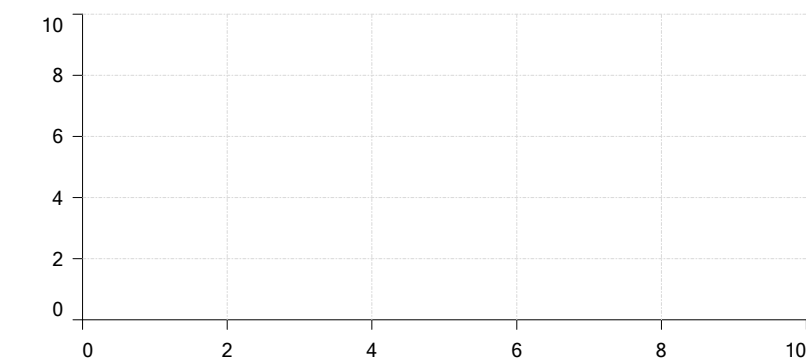
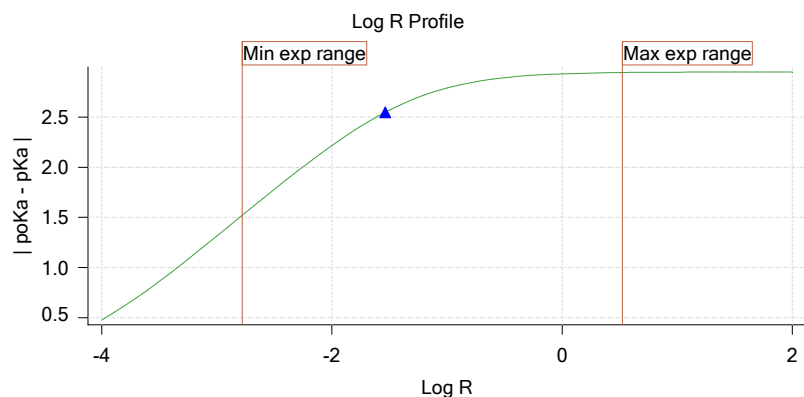
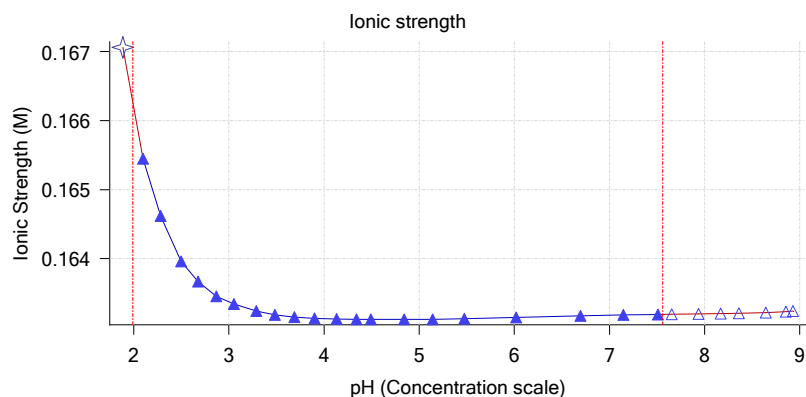
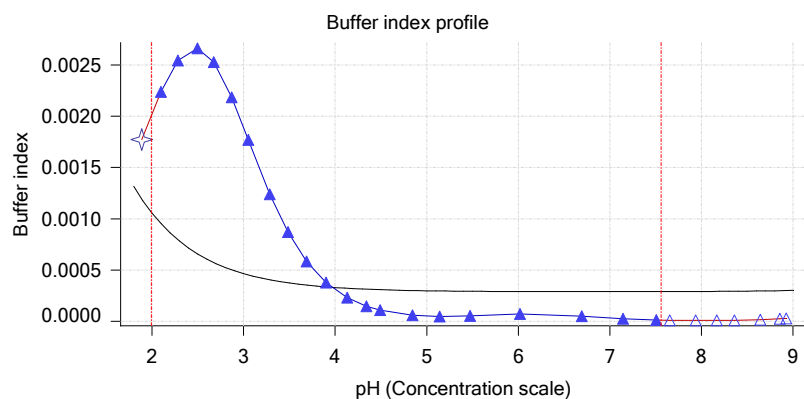
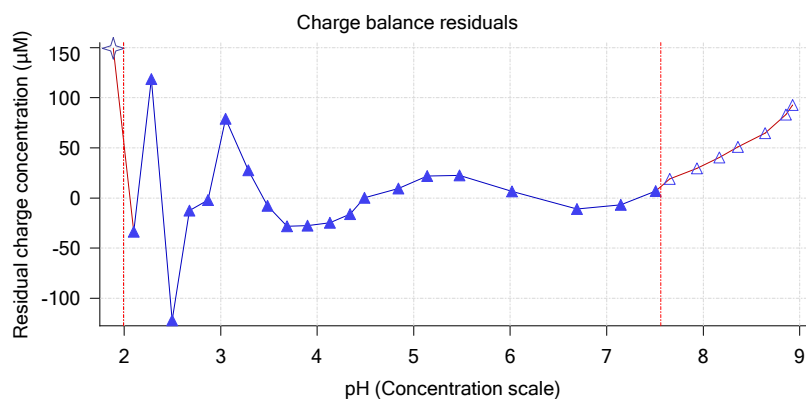
Other graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-03011 Points 49 to 70





Overall results

RMSD 0.256
 Average ionic strength 0.169 M
 Average temperature 25.0°C
 Partition ratio 0.1643 : 1
 Analyte concentration range 3175.3 µM to 3268.6 µM
 Total points considered 16 of 22



Warnings and errors

Errors None
 Warnings Sample concentration factor out of range
 Excessive acidity error present





Four-Plus parameters

 Alpha 0.111 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r

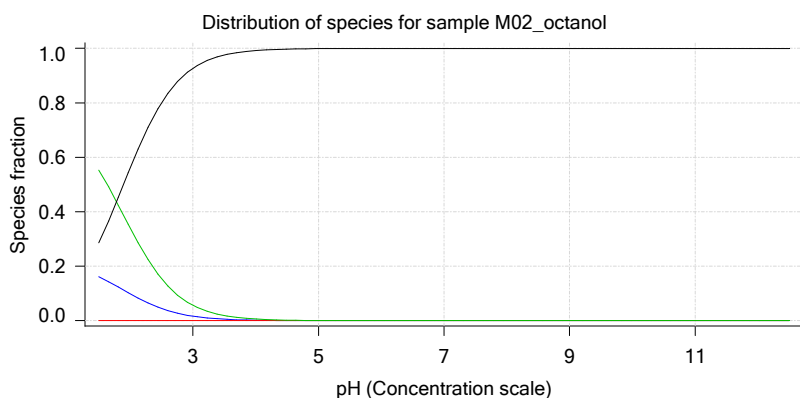
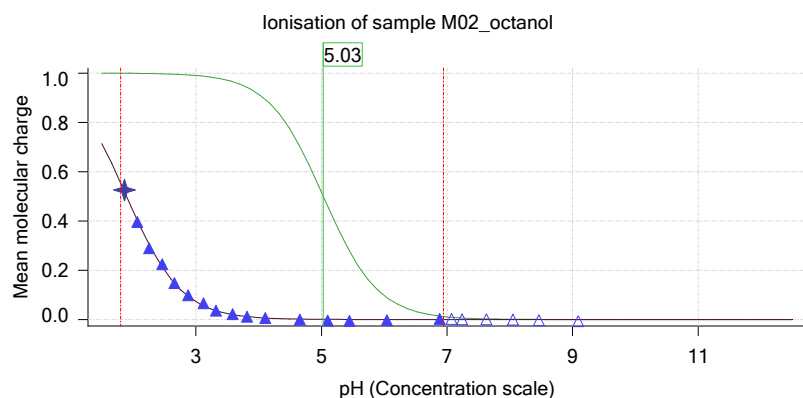
Titrants

 0.50 M HCl 0.999058 3/3/2018 1:46:01 PM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 1:46:01 PM C:\Sirius_T3\KOH18B27.t3r

Sample

 M02_octanol concentration factor 1.597
 Base pKa 1 5.03
 logP (XH +) 1.32
 logP (neutral X) 4.56

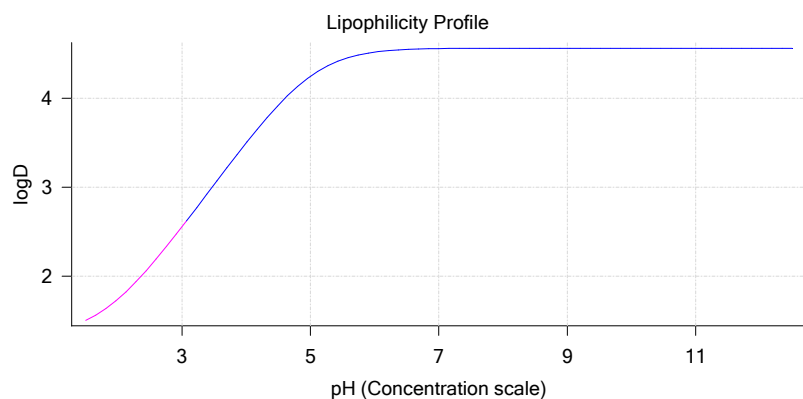
Sample graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Sample graphs (continued)



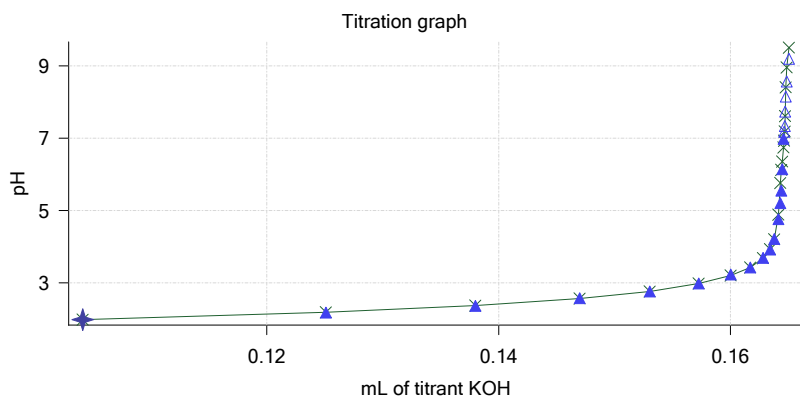
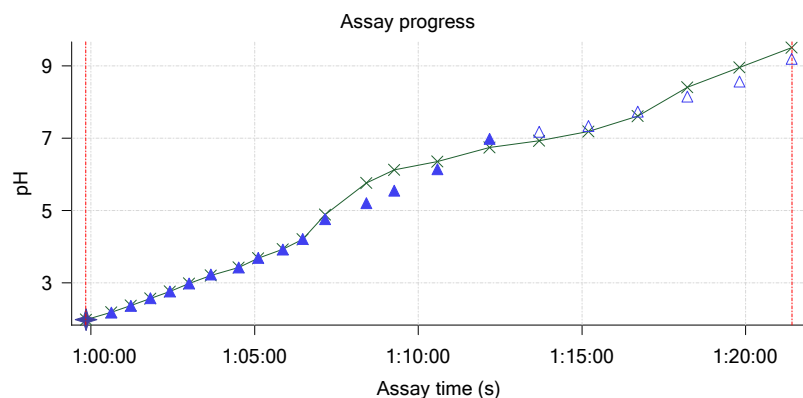
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanolH	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.39	20.02 %	0.00 %	68.72 %	11.26 %	Stomach pH
1.200	1.42	18.78 %	0.00 %	64.47 %	16.75 %	
2.000	1.74	9.94 %	0.01 %	34.13 %	55.92 %	
3.000	2.56	1.65 %	0.02 %	5.66 %	92.68 %	
4.000	3.50	0.18 %	0.02 %	0.61 %	99.20 %	
5.000	4.25	0.02 %	0.02 %	0.06 %	99.90 %	Blood pH
6.000	4.52	0.00 %	0.02 %	0.01 %	99.98 %	
6.500	4.55	0.00 %	0.02 %	0.00 %	99.98 %	
7.000	4.56	0.00 %	0.02 %	0.00 %	99.98 %	
7.400	4.56	0.00 %	0.02 %	0.00 %	99.98 %	
8.000	4.56	0.00 %	0.02 %	0.00 %	99.98 %	
9.000	4.56	0.00 %	0.02 %	0.00 %	99.98 %	
10.000	4.56	0.00 %	0.02 %	0.00 %	99.98 %	
11.000	4.56	0.00 %	0.02 %	0.00 %	99.98 %	
12.000	4.56	0.00 %	0.02 %	0.00 %	99.98 %	

Carbonate and acidity

Carbonate 0.148 mM
 Acidity error -1.252 mM

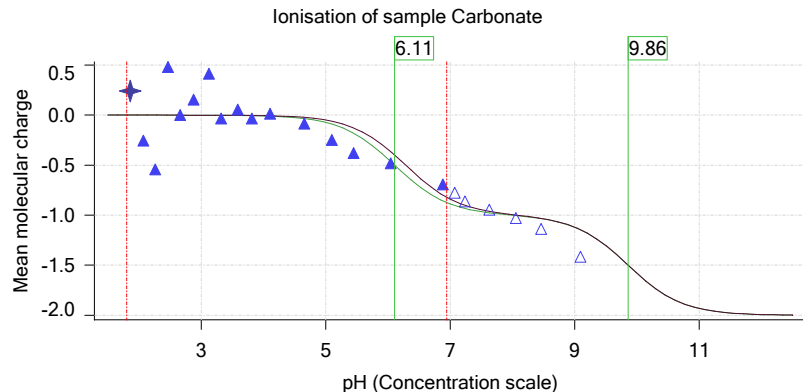
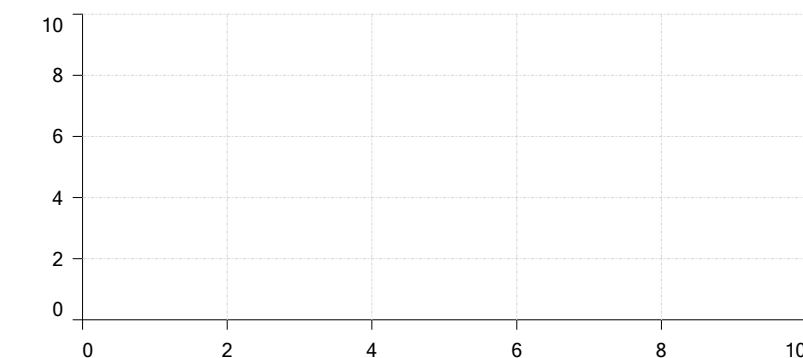
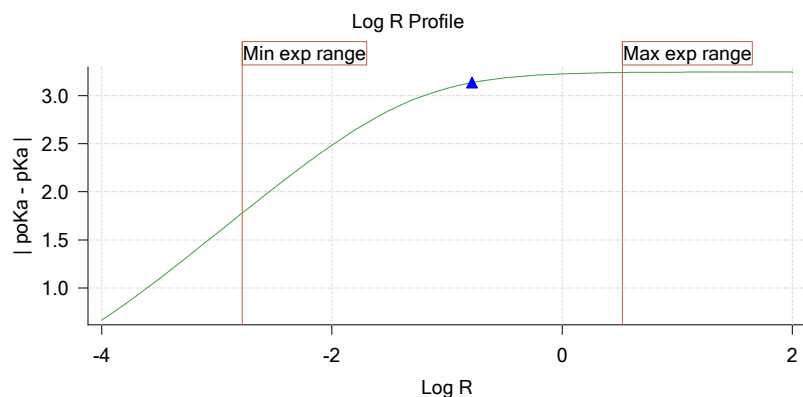
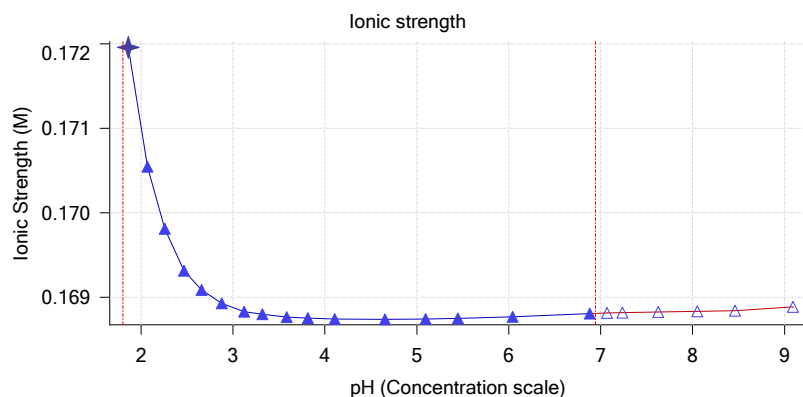
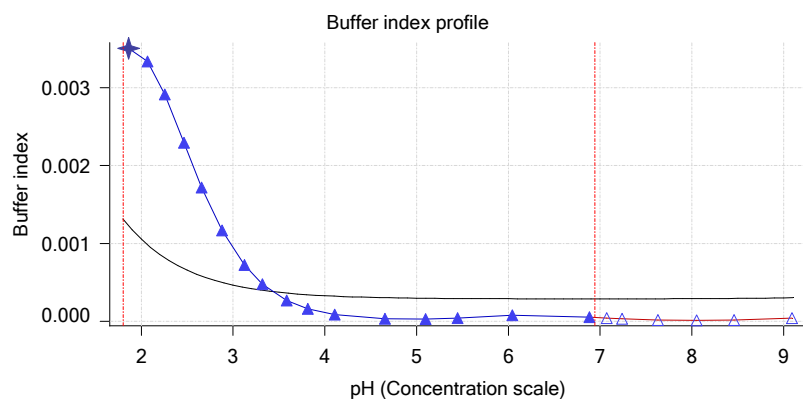
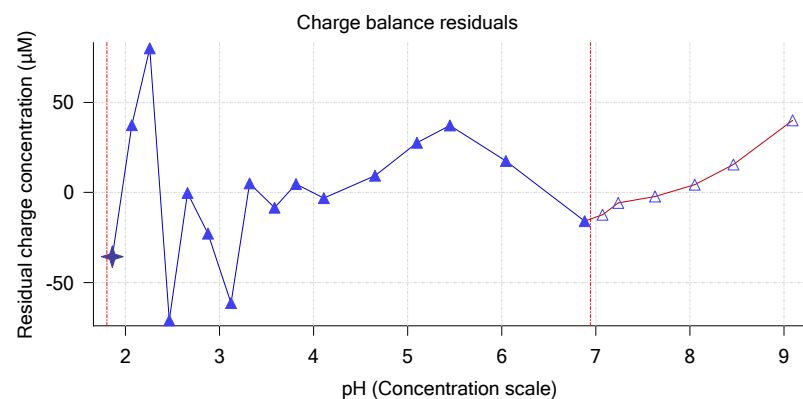
Other graphs



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M02_octanol	12/6/2017 4:20:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001960 g	3/2/2018 5:09:57 PM	User entered value
Formula weight	289.26 g/mol	12/6/2017 4:20:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	289.26	12/6/2017 4:20:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	12/6/2017 4:20:03 PM	User entered value
Sample is a	Base	12/6/2017 4:20:03 PM	User entered value
pKa 1	5.03	12/6/2017 4:20:03 PM	User entered value
logp (XH +)	1.32	3/2/2018 3:38:13 PM	User entered value
logP (neutral X)	4.10	3/2/2018 3:38:07 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
6:00.1	Initial pH = 8.70									
8:59.7	Data point 1	1.50000 mL	0.05252 mL	0.00162 mL	0.01999 mL	2.078	0.01636	0.75364	0.00093	15.0 s
9:50.7	Data point 2	1.50000 mL	0.05252 mL	0.01552 mL	0.01999 mL	2.285	-0.01511	0.81500	0.00083	10.5 s
10:26.8	Data point 3	1.50000 mL	0.05252 mL	0.02427 mL	0.01999 mL	2.490	-0.00148	0.44552	0.00011	10.5 s
11:02.9	Data point 4	1.50000 mL	0.05252 mL	0.03032 mL	0.01999 mL	2.678	-0.00348	0.65646	0.00021	10.0 s
11:38.4	Data point 5	1.50000 mL	0.05252 mL	0.03488 mL	0.01999 mL	2.876	-0.01455	0.84506	0.00078	10.0 s
12:13.9	Data point 6	1.50000 mL	0.05252 mL	0.03843 mL	0.01999 mL	3.094	-0.01527	0.85358	0.00082	10.5 s
12:49.9	Data point 7	1.50000 mL	0.05252 mL	0.04116 mL	0.01999 mL	3.288	-0.01663	0.96111	0.00084	10.0 s
13:25.4	Data point 8	1.50000 mL	0.05252 mL	0.04327 mL	0.01999 mL	3.515	-0.01850	0.86172	0.00098	23.0 s
14:13.9	Data point 9	1.50000 mL	0.05252 mL	0.04478 mL	0.01999 mL	3.760	-0.01848	0.86901	0.00098	17.0 s
15:11.8	Data point 10	1.50000 mL	0.05252 mL	0.04626 mL	0.01999 mL	4.096	-0.01860	0.90784	0.00096	20.0 s
16:12.8	Data point 11	1.50000 mL	0.05252 mL	0.04704 mL	0.01999 mL	4.437	-0.01860	0.90771	0.00096	37.5 s
17:20.9	Data point 12	1.50000 mL	0.05252 mL	0.04751 mL	0.01999 mL	4.850	-0.01809	0.87203	0.00096	43.0 s
18:34.5	Data point 13	1.50000 mL	0.05252 mL	0.04770 mL	0.01999 mL	5.134	-0.01884	0.90212	0.00098	51.0 s
19:56.1	Data point 14	1.50000 mL	0.05252 mL	0.04786 mL	0.01999 mL	5.651	-0.02196	0.93556	0.00112	Timed out at 59.5 s
21:31.8	Data point 15	1.50000 mL	0.05252 mL	0.04800 mL	0.01999 mL	6.482	-0.04707	0.98476	0.00234	Timed out at 59.5 s
23:07.4	Data point 16	1.50000 mL	0.05252 mL	0.04809 mL	0.01999 mL	6.961	-0.05553	0.98035	0.00277	Timed out at 59.5 s
24:38.0	Data point 17	1.50000 mL	0.05252 mL	0.04817 mL	0.01999 mL	7.521	-0.08676	0.99361	0.00430	Timed out at 59.5 s
26:13.5	Data point 18	1.50000 mL	0.05252 mL	0.04824 mL	0.01999 mL	8.125	-0.07978	0.98996	0.00396	Timed out at 59.5 s
27:49.3	Data point 19	1.50000 mL	0.05252 mL	0.04840 mL	0.01999 mL	8.917	-0.01848	0.88522	0.00097	56.0 s
29:15.8	Data point 20	1.50000 mL	0.05252 mL	0.04847 mL	0.01999 mL	9.138	-0.01766	0.91576	0.00091	37.0 s
30:51.7	Data point 21	1.50000 mL	0.10875 mL	0.04847 mL	0.05000 mL	2.009	-0.00919	0.60040	0.00059	10.0 s
31:38.0	Data point 22	1.50000 mL	0.10875 mL	0.06552 mL	0.05000 mL	2.215	-0.00727	0.64690	0.00045	10.0 s
32:13.7	Data point 23	1.50000 mL	0.10875 mL	0.07660 mL	0.05000 mL	2.396	-0.00146	0.31714	0.00013	10.5 s
32:49.9	Data point 24	1.50000 mL	0.10875 mL	0.08448 mL	0.05000 mL	2.609	-0.00346	0.43326	0.00026	10.0 s
33:25.5	Data point 25	1.50000 mL	0.10875 mL	0.08998 mL	0.05000 mL	2.785	-0.00991	0.29494	0.00090	10.0 s
34:01.0	Data point 26	1.50000 mL	0.10875 mL	0.09414 mL	0.05000 mL	2.978	-0.00636	0.79094	0.00035	10.0 s
34:36.5	Data point 27	1.50000 mL	0.10875 mL	0.09722 mL	0.05000 mL	3.160	-0.00652	0.78690	0.00036	10.0 s
35:11.9	Data point 28	1.50000 mL	0.10875 mL	0.09951 mL	0.05000 mL	3.395	-0.01414	0.94922	0.00072	10.5 s
36:03.3	Data point 29	1.50000 mL	0.10875 mL	0.10073 mL	0.05000 mL	3.592	-0.01172	0.70688	0.00069	10.0 s
36:54.3	Data point 30	1.50000 mL	0.10875 mL	0.10158 mL	0.05000 mL	3.795	-0.01307	0.64357	0.00080	10.0 s
37:45.1	Data point 31	1.50000 mL	0.10875 mL	0.10219 mL	0.05000 mL	4.005	-0.01735	0.75875	0.00098	10.5 s
38:21.1	Data point 32	1.50000 mL	0.10875 mL	0.10261 mL	0.05000 mL	4.238	-0.01660	0.84161	0.00089	12.5 s
38:59.1	Data point 33	1.50000 mL	0.10875 mL	0.10287 mL	0.05000 mL	4.447	-0.01934	0.93729	0.00099	16.0 s
39:40.4	Data point 34	1.50000 mL	0.10875 mL	0.10303 mL	0.05000 mL	4.596	-0.01901	0.88676	0.00100	30.5 s
40:41.5	Data point 35	1.50000 mL	0.10875 mL	0.10322 mL	0.05000 mL	4.948	-0.01691	0.77907	0.00095	16.0 s



Assay Events

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03011**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
41:28.0	Data point 36	1.50000 mL	0.10875 mL	0.10334 mL	0.05000 mL	5.244	-0.01809	0.82366	0.00098	32.5 s
42:31.1	Data point 37	1.50000 mL	0.10875 mL	0.10341 mL	0.05000 mL	5.578	-0.01894	0.89362	0.00099	47.0 s
43:48.7	Data point 38	1.50000 mL	0.10875 mL	0.10348 mL	0.05000 mL	6.124	-0.02064	0.93374	0.00106	Timed out at 59.5 s
45:19.2	Data point 39	1.50000 mL	0.10875 mL	0.10358 mL	0.05000 mL	6.796	-0.05867	0.98597	0.00292	Timed out at 59.5 s
46:54.9	Data point 40	1.50000 mL	0.10875 mL	0.10365 mL	0.05000 mL	7.247	-0.06483	0.98904	0.00322	Timed out at 59.5 s
48:30.7	Data point 41	1.50000 mL	0.10875 mL	0.10372 mL	0.05000 mL	7.610	-0.08577	0.99139	0.00426	Timed out at 59.5 s
50:01.2	Data point 42	1.50000 mL	0.10875 mL	0.10376 mL	0.05000 mL	7.754	-0.06230	0.98106	0.00311	Timed out at 59.5 s
51:31.7	Data point 43	1.50000 mL	0.10875 mL	0.10381 mL	0.05000 mL	8.038	-0.05883	0.98974	0.00292	Timed out at 59.5 s
53:02.2	Data point 44	1.50000 mL	0.10875 mL	0.10386 mL	0.05000 mL	8.269	-0.04245	0.97500	0.00212	Timed out at 59.5 s
54:32.7	Data point 45	1.50000 mL	0.10875 mL	0.10390 mL	0.05000 mL	8.461	-0.02925	0.94322	0.00149	Timed out at 59.5 s
56:08.3	Data point 46	1.50000 mL	0.10875 mL	0.10398 mL	0.05000 mL	8.742	-0.01524	0.61499	0.00096	30.5 s
57:14.5	Data point 47	1.50000 mL	0.10875 mL	0.10407 mL	0.05000 mL	8.956	-0.01863	0.86242	0.00099	36.0 s
58:21.1	Data point 48	1.50000 mL	0.10875 mL	0.10412 mL	0.05000 mL	9.027	-0.01667	0.74240	0.00096	26.0 s
59:51.2	Data point 49	1.50000 mL	0.16893 mL	0.10412 mL	0.30000 mL	1.983	0.00363	0.07579	0.00065	10.0 s
1:00:37.5	Data point 50	1.50000 mL	0.16893 mL	0.12509 mL	0.30000 mL	2.185	-0.01327	0.52474	0.00091	10.0 s
1:01:13.3	Data point 51	1.50000 mL	0.16893 mL	0.13801 mL	0.30000 mL	2.371	-0.01259	0.50607	0.00087	10.0 s
1:01:48.9	Data point 52	1.50000 mL	0.16893 mL	0.14699 mL	0.30000 mL	2.577	-0.00872	0.34259	0.00074	10.0 s
1:02:24.5	Data point 53	1.50000 mL	0.16893 mL	0.15303 mL	0.30000 mL	2.768	-0.00055	0.00118	0.00079	10.0 s
1:02:59.9	Data point 54	1.50000 mL	0.16893 mL	0.15727 mL	0.30000 mL	2.987	-0.00399	0.04207	0.00096	14.5 s
1:03:39.9	Data point 55	1.50000 mL	0.16893 mL	0.16002 mL	0.30000 mL	3.230	-0.00293	0.03061	0.00083	10.0 s
1:04:30.9	Data point 56	1.50000 mL	0.16893 mL	0.16169 mL	0.30000 mL	3.426	0.01036	0.28200	0.00096	10.0 s
1:05:06.3	Data point 57	1.50000 mL	0.16893 mL	0.16279 mL	0.30000 mL	3.692	-0.01047	0.32693	0.00090	15.0 s
1:05:51.9	Data point 58	1.50000 mL	0.16893 mL	0.16340 mL	0.30000 mL	3.919	-0.00471	0.52606	0.00032	10.5 s
1:06:27.8	Data point 59	1.50000 mL	0.16893 mL	0.16378 mL	0.30000 mL	4.213	-0.01245	0.91405	0.00064	10.5 s
1:07:09.1	Data point 60	1.50000 mL	0.16893 mL	0.16414 mL	0.30000 mL	4.759	-0.01882	0.91127	0.00097	45.0 s
1:08:24.9	Data point 61	1.50000 mL	0.16893 mL	0.16430 mL	0.30000 mL	5.201	-0.01315	0.55571	0.00087	15.5 s
1:09:16.0	Data point 62	1.50000 mL	0.16893 mL	0.16439 mL	0.30000 mL	5.551	-0.01841	0.93035	0.00094	48.5 s
1:10:35.1	Data point 63	1.50000 mL	0.16893 mL	0.16446 mL	0.30000 mL	6.146	-0.03968	0.91076	0.00205	Timed out at 59.5 s
1:12:10.7	Data point 64	1.50000 mL	0.16893 mL	0.16458 mL	0.30000 mL	6.984	-0.09924	0.98030	0.00495	Timed out at 59.5 s
1:13:41.3	Data point 65	1.50000 mL	0.16893 mL	0.16463 mL	0.30000 mL	7.173	-0.07212	0.97043	0.00362	Timed out at 59.5 s
1:15:11.8	Data point 66	1.50000 mL	0.16893 mL	0.16467 mL	0.30000 mL	7.339	-0.06600	0.98427	0.00328	Timed out at 59.5 s
1:16:42.3	Data point 67	1.50000 mL	0.16893 mL	0.16472 mL	0.30000 mL	7.729	-0.07810	0.99269	0.00387	Timed out at 59.5 s
1:18:12.8	Data point 68	1.50000 mL	0.16893 mL	0.16477 mL	0.30000 mL	8.153	-0.05661	0.98395	0.00282	Timed out at 59.5 s
1:19:48.4	Data point 69	1.50000 mL	0.16893 mL	0.16484 mL	0.30000 mL	8.561	-0.03628	0.93717	0.00185	Timed out at 59.5 s
1:21:24.0	Data point 70	1.50000 mL	0.16893 mL	0.16505 mL	0.30000 mL	9.190	-0.01034	0.34587	0.00087	15.0 s
1:21:48.1	Assay volumes	1.50000 mL	0.16893 mL	0.16505 mL	0.30000 mL					

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.030 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M02_octanol** Experiment start time: **3/3/2018 1:46:01 PM**
 Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
 Assay ID: **18C-03011** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.250 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/3/2018 1:46:01 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/3/2018 1:46:01 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/3/2018 1:46:01 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/3/2018 1:46:01 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/3/2018 1:46:01 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/3/2018 1:46:01 PM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titration		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+6.59 mV		3/3/2018 1:46:29 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Triton X-100 in H2O		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	6.7e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.7e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M02_octanol** Experiment start time: **3/3/2018 1:46:01 PM**
 Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
 Assay ID: **18C-03011** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:38] Air gap created for Water (0.15 M KCl)
 [2:38] Air gap created for Acid (0.5 M HCl)
 [2:38] Air gap created for Base (0.5 M KOH)
 [2:39] Air gap released for Water (0.15 M KCl)
 [2:42] Titrator arm moved over Titration position
 [2:42] Titration 1 of 3
 [2:42] Adding initial titrants
 [2:42] Automatically add 1.50000 mL of water
 [3:08] Dispensed 1.500000 mL of Water (0.15 M KCl)
 [3:12] Titrator arm moved over Drain
 [5:54] Titrator arm moved to Titration position
 [5:54] Argon flow rate set to 100
 [5:54] Stirrer speed set to 10
 [5:59] Automatically add 0.02000 mL of Octanol
 [5:59] Dispensed 0.019991 mL of Octanol
 [6:00] Initial pH = 8.70
 [6:00] Iterative adjust 8.70 -> 2.00
 [6:00] pH 8.70 -> 2.00
 [6:02] Air gap released for Acid (0.5 M HCl)
 [6:03] Dispensed 0.052516 mL of Acid (0.5 M HCl)
 [6:08] Holding pH 2.00
 [8:08] Stirrer speed set to 0
 [8:08] Stirrer speed set to 50
 [8:08] Iterative adjust 1.98 -> 2.00
 [8:08] pH 1.98 -> 2.00
 [8:09] Air gap released for Base (0.5 M KOH)
 [8:10] Dispensed 0.001623 mL of Base (0.5 M KOH)
 [9:00] Stirrer speed set to 0
 [9:15] Datapoint id 1 collected
 [9:15] Stirrer speed set to 50
 [9:20] pH 2.08 -> 2.28
 [9:20] Using cautious pH adjust
 [9:20] Dispensed 0.006656 mL of Base (0.5 M KOH)
 [9:25] Stepping pH = 2.17
 [9:26] Dispensed 0.005456 mL of Base (0.5 M KOH)
 [9:31] Stepping pH = 2.25
 [9:31] Dispensed 0.001787 mL of Base (0.5 M KOH)
 [9:36] Stepping pH = 2.29
 [9:51] Stirrer speed set to 0
 [10:02] Datapoint id 2 collected
 [10:02] Charge balance equation is out by -4.4%
 [10:02] Stirrer speed set to 50

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Experiment Log (continued)

[10:07] pH 2.29 -> 2.49
 [10:07] Using charge balance adjust
 [10:07] Dispensed 0.008749 mL of Base (0.5 M KOH)
 [10:27] Stirrer speed set to 0
 [10:38] Datapoint id 3 collected
 [10:38] Charge balance equation is out by -0.3%
 [10:38] Stirrer speed set to 50
 [10:43] pH 2.50 -> 2.70
 [10:43] Using charge balance adjust
 [10:43] Dispensed 0.006044 mL of Base (0.5 M KOH)
 [11:03] Stirrer speed set to 0
 [11:13] Datapoint id 4 collected
 [11:13] Charge balance equation is out by -8.9%
 [11:13] Stirrer speed set to 50
 [11:18] pH 2.68 -> 2.88
 [11:18] Using charge balance adjust
 [11:19] Dispensed 0.004563 mL of Base (0.5 M KOH)
 [11:39] Stirrer speed set to 0
 [11:49] Datapoint id 5 collected
 [11:49] Charge balance equation is out by -3.6%
 [11:49] Stirrer speed set to 50
 [11:54] pH 2.88 -> 3.08
 [11:54] Using charge balance adjust
 [11:54] Dispensed 0.003551 mL of Base (0.5 M KOH)
 [12:14] Stirrer speed set to 0
 [12:25] Datapoint id 6 collected
 [12:25] Charge balance equation is out by 8.3%
 [12:25] Stirrer speed set to 50
 [12:30] pH 3.10 -> 3.30
 [12:30] Using charge balance adjust
 [12:30] Dispensed 0.002728 mL of Base (0.5 M KOH)
 [12:50] Stirrer speed set to 0
 [13:00] Datapoint id 7 collected
 [13:00] Charge balance equation is out by -4.3%
 [13:00] Stirrer speed set to 50
 [13:05] pH 3.29 -> 3.49
 [13:05] Using charge balance adjust
 [13:06] Dispensed 0.002117 mL of Base (0.5 M KOH)
 [13:26] Stirrer speed set to 0
 [13:49] Datapoint id 8 collected
 [13:49] Charge balance equation is out by 12.1%
 [13:49] Stirrer speed set to 50
 [13:54] pH 3.51 -> 3.71
 [13:54] Using charge balance adjust
 [13:54] Dispensed 0.001505 mL of Base (0.5 M KOH)
 [14:14] Stirrer speed set to 0
 [14:31] Datapoint id 9 collected
 [14:31] Charge balance equation is out by 23.9%
 [14:31] Stirrer speed set to 50
 [14:36] pH 3.76 -> 3.96
 [14:36] Using cautious pH adjust
 [14:36] Dispensed 0.000494 mL of Base (0.5 M KOH)
 [14:42] Stepping pH = 3.86
 [14:42] Dispensed 0.000306 mL of Base (0.5 M KOH)
 [14:47] Stepping pH = 3.94
 [14:47] Dispensed 0.000047 mL of Base (0.5 M KOH)
 [14:52] Stepping pH = 3.92
 [14:52] Dispensed 0.000635 mL of Base (0.5 M KOH)
 [14:57] Stepping pH = 4.16

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03011**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[15:12] Stirrer speed set to 0
[15:32] Datapoint id 10 collected
[15:32] Charge balance equation is out by -51.7%
[15:32] Stirrer speed set to 50
[15:37] pH 4.11 -> 4.31
[15:37] Using cautious pH adjust
[15:37] Dispensed 0.000259 mL of Base (0.5 M KOH)
[15:42] Stepping pH = 4.20
[15:43] Dispensed 0.000188 mL of Base (0.5 M KOH)
[15:48] Stepping pH = 4.28
[15:48] Dispensed 0.000047 mL of Base (0.5 M KOH)
[15:53] Stepping pH = 4.28
[15:53] Dispensed 0.000282 mL of Base (0.5 M KOH)
[15:58] Stepping pH = 4.50
[16:13] Stirrer speed set to 0
[16:51] Datapoint id 11 collected
[16:51] Charge balance equation is out by -54.0%
[16:51] Stirrer speed set to 50
[16:56] pH 4.45 -> 4.65
[16:56] Using cautious pH adjust
[16:56] Dispensed 0.000118 mL of Base (0.5 M KOH)
[17:01] Stepping pH = 4.46
[17:01] Dispensed 0.000353 mL of Base (0.5 M KOH)
[17:06] Stepping pH = 4.97
[17:21] Stirrer speed set to 0
[18:04] Datapoint id 12 collected
[18:04] Charge balance equation is out by -97.0%
[18:04] Stirrer speed set to 50
[18:09] pH 4.93 -> 5.13
[18:09] Using cautious pH adjust
[18:09] Dispensed 0.000047 mL of Base (0.5 M KOH)
[18:15] Stepping pH = 4.94
[18:15] Dispensed 0.000141 mL of Base (0.5 M KOH)
[18:20] Stepping pH = 5.22
[18:35] Stirrer speed set to 0
[19:26] Datapoint id 13 collected
[19:26] Charge balance equation is out by -95.2%
[19:26] Stirrer speed set to 50
[19:31] pH 5.23 -> 5.43
[19:31] Using cautious pH adjust
[19:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[19:36] Stepping pH = 5.23
[19:36] Dispensed 0.000141 mL of Base (0.5 M KOH)
[19:41] Stepping pH = 5.64
[19:56] Stirrer speed set to 0
[20:56] Datapoint id 14 collected
[20:56] Charge balance equation is out by -204.5%
[20:56] Stirrer speed set to 50
[21:02] pH 5.71 -> 5.91
[21:02] Using cautious pH adjust
[21:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:07] Stepping pH = 5.75
[21:07] Dispensed 0.000047 mL of Base (0.5 M KOH)
[21:12] Stepping pH = 5.78
[21:12] Dispensed 0.000071 mL of Base (0.5 M KOH)
[21:17] Stepping pH = 6.41
[21:32] Stirrer speed set to 0
[22:32] Datapoint id 15 collected
[22:32] Charge balance equation is out by -213.0%

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03011**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[22:32] Stirrer speed set to 50
[22:37] pH 6.50 -> 6.70
[22:37] Using cautious pH adjust
[22:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:42] Stepping pH = 6.50
[22:42] Dispensed 0.000047 mL of Base (0.5 M KOH)
[22:47] Stepping pH = 6.64
[22:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:53] Stepping pH = 6.88
[23:08] Stirrer speed set to 0
[24:08] Datapoint id 16 collected
[24:08] Charge balance equation is out by -164.9%
[24:08] Stirrer speed set to 50
[24:13] pH 6.94 -> 7.14
[24:13] Using cautious pH adjust
[24:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:18] Stepping pH = 6.91
[24:18] Dispensed 0.000047 mL of Base (0.5 M KOH)
[24:23] Stepping pH = 7.15
[24:38] Stirrer speed set to 0
[25:38] Datapoint id 17 collected
[25:38] Charge balance equation is out by -314.2%
[25:38] Stirrer speed set to 50
[25:43] pH 7.53 -> 7.73
[25:43] Using cautious pH adjust
[25:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:49] Stepping pH = 7.51
[25:49] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:54] Stepping pH = 7.55
[25:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:59] Stepping pH = 7.84
[26:14] Stirrer speed set to 0
[27:14] Datapoint id 18 collected
[27:14] Charge balance equation is out by -916.6%
[27:14] Stirrer speed set to 50
[27:19] pH 8.10 -> 8.30
[27:19] Using cautious pH adjust
[27:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:24] Stepping pH = 8.05
[27:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:29] Stepping pH = 8.01
[27:29] Dispensed 0.000118 mL of Base (0.5 M KOH)
[27:35] Stepping pH = 8.98
[27:50] Stirrer speed set to 0
[28:46] Datapoint id 19 collected
[28:46] Charge balance equation is out by -2,236.6%
[28:46] Stirrer speed set to 50
[28:51] pH 8.92 -> 9.05
[28:51] Using cautious pH adjust
[28:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:56] Stepping pH = 8.92
[28:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
[29:01] Stepping pH = 9.11
[29:16] Stirrer speed set to 0
[29:53] Datapoint id 20 collected
[29:53] Charge balance equation is out by -259.1%
[29:53] Titration 2 of 3
[29:53] Adding initial titrants
[29:53] Automatically add 0.03000 mL of Octanol

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03011**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[29:54] Dispensed 0.030009 mL of Octanol
[29:54] Stirrer speed set to 10
[29:55] Stirrer speed set to 55
[29:55] Iterative adjust 9.14 -> 2.00
[29:55] pH 9.14 -> 2.00
[29:57] Dispensed 0.054492 mL of Acid (0.5 M HCl)
[30:02] pH 2.02 -> 2.00
[30:02] Dispensed 0.001740 mL of Acid (0.5 M HCl)
[30:52] Stirrer speed set to 0
[31:02] Datapoint id 21 collected
[31:02] Stirrer speed set to 55
[31:07] pH 2.02 -> 2.22
[31:07] Using cautious pH adjust
[31:08] Dispensed 0.008396 mL of Base (0.5 M KOH)
[31:13] Stepping pH = 2.10
[31:13] Dispensed 0.007079 mL of Base (0.5 M KOH)
[31:18] Stepping pH = 2.19
[31:18] Dispensed 0.001576 mL of Base (0.5 M KOH)
[31:23] Stepping pH = 2.21
[31:38] Stirrer speed set to 0
[31:48] Datapoint id 22 collected
[31:48] Charge balance equation is out by -1.5%
[31:48] Stirrer speed set to 55
[31:54] pH 2.22 -> 2.42
[31:54] Using charge balance adjust
[31:54] Dispensed 0.011077 mL of Base (0.5 M KOH)
[32:14] Stirrer speed set to 0
[32:25] Datapoint id 23 collected
[32:25] Charge balance equation is out by -11.5%
[32:25] Stirrer speed set to 55
[32:30] pH 2.40 -> 2.60
[32:30] Using charge balance adjust
[32:30] Dispensed 0.007879 mL of Base (0.5 M KOH)
[32:50] Stirrer speed set to 0
[33:00] Datapoint id 24 collected
[33:00] Charge balance equation is out by 4.0%
[33:00] Stirrer speed set to 55
[33:05] pH 2.61 -> 2.81
[33:05] Using charge balance adjust
[33:06] Dispensed 0.005503 mL of Base (0.5 M KOH)
[33:26] Stirrer speed set to 0
[33:36] Datapoint id 25 collected
[33:36] Charge balance equation is out by -14.7%
[33:36] Stirrer speed set to 55
[33:41] pH 2.79 -> 2.99
[33:41] Using charge balance adjust
[33:41] Dispensed 0.004163 mL of Base (0.5 M KOH)
[34:01] Stirrer speed set to 0
[34:11] Datapoint id 26 collected
[34:11] Charge balance equation is out by -5.7%
[34:11] Stirrer speed set to 55
[34:16] pH 2.98 -> 3.18
[34:16] Using charge balance adjust
[34:17] Dispensed 0.003081 mL of Base (0.5 M KOH)
[34:37] Stirrer speed set to 0
[34:47] Datapoint id 27 collected
[34:47] Charge balance equation is out by -10.6%
[34:47] Stirrer speed set to 55
[34:52] pH 3.16 -> 3.36

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03011**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[34:52] Using charge balance adjust
[34:52] Dispensed 0.002281 mL of Base (0.5 M KOH)
[35:12] Stirrer speed set to 0
[35:23] Datapoint id 28 collected
[35:23] Charge balance equation is out by 15.1%
[35:23] Stirrer speed set to 55
[35:28] pH 3.40 -> 3.60
[35:28] Using cautious pH adjust
[35:28] Dispensed 0.000753 mL of Base (0.5 M KOH)
[35:33] Stepping pH = 3.52
[35:33] Dispensed 0.000306 mL of Base (0.5 M KOH)
[35:38] Stepping pH = 3.58
[35:38] Dispensed 0.000047 mL of Base (0.5 M KOH)
[35:43] Stepping pH = 3.59
[35:43] Dispensed 0.000118 mL of Base (0.5 M KOH)
[35:49] Stepping pH = 3.61
[36:04] Stirrer speed set to 0
[36:14] Datapoint id 29 collected
[36:14] Charge balance equation is out by 17.7%
[36:14] Stirrer speed set to 55
[36:19] pH 3.60 -> 3.80
[36:19] Using cautious pH adjust
[36:19] Dispensed 0.000517 mL of Base (0.5 M KOH)
[36:24] Stepping pH = 3.73
[36:24] Dispensed 0.000188 mL of Base (0.5 M KOH)
[36:29] Stepping pH = 3.77
[36:29] Dispensed 0.000071 mL of Base (0.5 M KOH)
[36:34] Stepping pH = 3.78
[36:34] Dispensed 0.000071 mL of Base (0.5 M KOH)
[36:40] Stepping pH = 3.80
[36:55] Stirrer speed set to 0
[37:05] Datapoint id 30 collected
[37:05] Charge balance equation is out by 16.3%
[37:05] Stirrer speed set to 55
[37:10] pH 3.80 -> 4.00
[37:10] Using cautious pH adjust
[37:10] Dispensed 0.000329 mL of Base (0.5 M KOH)
[37:15] Stepping pH = 3.91
[37:15] Dispensed 0.000188 mL of Base (0.5 M KOH)
[37:20] Stepping pH = 3.99
[37:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:25] Stepping pH = 3.99
[37:25] Dispensed 0.000071 mL of Base (0.5 M KOH)
[37:30] Stepping pH = 4.02
[37:45] Stirrer speed set to 0
[37:56] Datapoint id 31 collected
[37:56] Charge balance equation is out by 9.2%
[37:56] Stirrer speed set to 55
[38:01] pH 4.02 -> 4.22
[38:01] Using charge balance adjust
[38:01] Dispensed 0.000423 mL of Base (0.5 M KOH)
[38:21] Stirrer speed set to 0
[38:34] Datapoint id 32 collected
[38:34] Charge balance equation is out by 10.4%
[38:34] Stirrer speed set to 55
[38:39] pH 4.26 -> 4.46
[38:39] Using charge balance adjust
[38:39] Dispensed 0.000259 mL of Base (0.5 M KOH)
[38:59] Stirrer speed set to 0

Sample name: **M02_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03011**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Experiment Log (continued)

[39:15] Datapoint id 33 collected
 [39:15] Charge balance equation is out by -4.0%
 [39:15] Stirrer speed set to 55
 [39:21] pH 4.47 -> 4.67
 [39:21] Using charge balance adjust
 [39:21] Dispensed 0.000165 mL of Base (0.5 M KOH)
 [39:41] Stirrer speed set to 0
 [40:11] Datapoint id 34 collected
 [40:11] Charge balance equation is out by -37.4%
 [40:11] Stirrer speed set to 55
 [40:16] pH 4.64 -> 4.84
 [40:16] Using cautious pH adjust
 [40:17] Dispensed 0.000047 mL of Base (0.5 M KOH)
 [40:22] Stepping pH = 4.65
 [40:22] Dispensed 0.000141 mL of Base (0.5 M KOH)
 [40:27] Stepping pH = 4.98
 [40:42] Stirrer speed set to 0
 [40:58] Datapoint id 35 collected
 [40:58] Charge balance equation is out by -87.0%
 [40:58] Stirrer speed set to 55
 [41:03] pH 5.00 -> 5.20
 [41:03] Using cautious pH adjust
 [41:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
 [41:08] Stepping pH = 5.00
 [41:08] Dispensed 0.000094 mL of Base (0.5 M KOH)
 [41:13] Stepping pH = 5.27
 [41:28] Stirrer speed set to 0
 [42:01] Datapoint id 36 collected
 [42:01] Charge balance equation is out by -98.9%
 [42:01] Stirrer speed set to 55
 [42:06] pH 5.33 -> 5.53
 [42:06] Using cautious pH adjust
 [42:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
 [42:11] Stepping pH = 5.34
 [42:11] Dispensed 0.000047 mL of Base (0.5 M KOH)
 [42:16] Stepping pH = 5.59
 [42:31] Stirrer speed set to 0
 [43:19] Datapoint id 37 collected
 [43:19] Charge balance equation is out by -92.9%
 [43:19] Stirrer speed set to 55
 [43:24] pH 5.70 -> 5.90
 [43:24] Using cautious pH adjust
 [43:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
 [43:29] Stepping pH = 5.72
 [43:29] Dispensed 0.000047 mL of Base (0.5 M KOH)
 [43:34] Stepping pH = 6.12
 [43:49] Stirrer speed set to 0
 [44:49] Datapoint id 38 collected
 [44:49] Charge balance equation is out by -87.7%
 [44:49] Stirrer speed set to 55
 [44:54] pH 6.16 -> 6.36
 [44:54] Using cautious pH adjust
 [44:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
 [44:59] Stepping pH = 6.16
 [44:59] Dispensed 0.000071 mL of Base (0.5 M KOH)
 [45:04] Stepping pH = 6.69
 [45:20] Stirrer speed set to 0
 [46:20] Datapoint id 39 collected
 [46:20] Charge balance equation is out by -96.1%

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03011**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03011_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 1:46:01 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[46:20] Stirrer speed set to 55
[46:25] pH 6.83 -> 7.03
[46:25] Using cautious pH adjust
[46:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[46:30] Stepping pH = 6.85
[46:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[46:35] Stepping pH = 6.96
[46:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[46:40] Stepping pH = 7.20
[46:55] Stirrer speed set to 0
[47:55] Datapoint id 40 collected
[47:55] Charge balance equation is out by -198.9%
[47:55] Stirrer speed set to 55
[48:00] pH 7.31 -> 7.51
[48:00] Using cautious pH adjust
[48:00] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:05] Stepping pH = 7.34
[48:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:11] Stepping pH = 7.46
[48:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:16] Stepping pH = 7.68
[48:31] Stirrer speed set to 0
[49:31] Datapoint id 41 collected
[49:31] Charge balance equation is out by -452.4%
[49:31] Stirrer speed set to 55
[49:36] pH 7.54 -> 7.74
[49:36] Using cautious pH adjust
[49:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:41] Stepping pH = 7.55
[49:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:46] Stepping pH = 7.73
[50:02] Stirrer speed set to 0
[51:02] Datapoint id 42 collected
[51:02] Charge balance equation is out by -414.6%
[51:02] Stirrer speed set to 55
[51:07] pH 7.69 -> 7.89
[51:07] Using cautious pH adjust
[51:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[51:12] Stepping pH = 7.66
[51:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[51:17] Stepping pH = 7.90
[51:32] Stirrer speed set to 0
[52:32] Datapoint id 43 collected
[52:32] Charge balance equation is out by -498.4%
[52:32] Stirrer speed set to 55
[52:37] pH 8.03 -> 8.23
[52:37] Using cautious pH adjust
[52:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:42] Stepping pH = 8.05
[52:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:47] Stepping pH = 8.24
[53:02] Stirrer speed set to 0
[54:03] Datapoint id 44 collected
[54:03] Charge balance equation is out by -454.8%
[54:03] Stirrer speed set to 55
[54:08] pH 8.27 -> 8.47
[54:08] Using cautious pH adjust
[54:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:13] Stepping pH = 8.30

Sample name: **M02_octanol**
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Experiment start time: **3/3/2018 1:46:01 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[54:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:18] Stepping pH = 8.46
[54:33] Stirrer speed set to 0
[55:33] Datapoint id 45 collected
[55:33] Charge balance equation is out by -298.4%
[55:33] Stirrer speed set to 55
[55:38] pH 8.50 -> 8.70
[55:38] Using cautious pH adjust
[55:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:43] Stepping pH = 8.53
[55:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:48] Stepping pH = 8.65
[55:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:54] Stepping pH = 8.76
[56:09] Stirrer speed set to 0
[56:39] Datapoint id 46 collected
[56:39] Charge balance equation is out by -284.7%
[56:39] Stirrer speed set to 55
[56:44] pH 8.74 -> 8.94
[56:44] Using cautious pH adjust
[56:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:49] Stepping pH = 8.74
[56:50] Dispensed 0.000047 mL of Base (0.5 M KOH)
[56:55] Stepping pH = 8.90
[56:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:00] Stepping pH = 8.96
[57:15] Stirrer speed set to 0
[57:51] Datapoint id 47 collected
[57:51] Charge balance equation is out by -204.3%
[57:51] Stirrer speed set to 55
[57:56] pH 8.98 -> 9.05
[57:56] Using cautious pH adjust
[57:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:01] Stepping pH = 8.98
[58:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:06] Stepping pH = 9.02
[58:21] Stirrer speed set to 0
[58:48] Datapoint id 48 collected
[58:48] Charge balance equation is out by -216.1%
[58:48] Titration 3 of 3
[58:48] Adding initial titrants
[58:48] Automatically add 0.25000 mL of Octanol
[58:53] Dispensed 0.250000 mL of Octanol
[58:53] Stirrer speed set to 10
[58:55] Stirrer speed set to 60
[58:55] Iterative adjust 9.03 -> 2.00
[58:55] pH 9.03 -> 2.00
[58:56] Dispensed 0.056044 mL of Acid (0.5 M HCl)
[59:01] pH 2.04 -> 2.00
[59:01] Dispensed 0.004139 mL of Acid (0.5 M HCl)
[59:52] Stirrer speed set to 0
[1:00:02] Datapoint id 49 collected
[1:00:02] Stirrer speed set to 60
[1:00:07] pH 1.99 -> 2.19
[1:00:07] Using cautious pH adjust
[1:00:07] Dispensed 0.009666 mL of Base (0.5 M KOH)
[1:00:12] Stepping pH = 2.07
[1:00:12] Dispensed 0.009055 mL of Base (0.5 M KOH)
[1:00:17] Stepping pH = 2.16

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Experiment start time: **3/3/2018 1:46:01 PM**
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Instrument ID: **T312060**

Experiment Log (continued)

[1:00:18] Dispensed 0.002258 mL of Base (0.5 M KOH)
[1:00:23] Stepping pH = 2.19
[1:00:38] Stirrer speed set to 0
[1:00:48] Datapoint id 50 collected
[1:00:48] Charge balance equation is out by -8.6%
[1:00:48] Stirrer speed set to 60
[1:00:53] pH 2.19 -> 2.39
[1:00:53] Using charge balance adjust
[1:00:53] Dispensed 0.012912 mL of Base (0.5 M KOH)
[1:01:14] Stirrer speed set to 0
[1:01:24] Datapoint id 51 collected
[1:01:24] Charge balance equation is out by -8.4%
[1:01:24] Stirrer speed set to 60
[1:01:29] pH 2.37 -> 2.57
[1:01:29] Using charge balance adjust
[1:01:29] Dispensed 0.008984 mL of Base (0.5 M KOH)
[1:01:49] Stirrer speed set to 0
[1:01:59] Datapoint id 52 collected
[1:01:59] Charge balance equation is out by 2.2%
[1:01:59] Stirrer speed set to 60
[1:02:04] pH 2.58 -> 2.78
[1:02:04] Using charge balance adjust
[1:02:05] Dispensed 0.006044 mL of Base (0.5 M KOH)
[1:02:25] Stirrer speed set to 0
[1:02:35] Datapoint id 53 collected
[1:02:35] Charge balance equation is out by -7.6%
[1:02:35] Stirrer speed set to 60
[1:02:40] pH 2.77 -> 2.97
[1:02:40] Using charge balance adjust
[1:02:40] Dispensed 0.004233 mL of Base (0.5 M KOH)
[1:03:00] Stirrer speed set to 0
[1:03:15] Datapoint id 54 collected
[1:03:15] Charge balance equation is out by 7.6%
[1:03:15] Stirrer speed set to 60
[1:03:20] pH 2.99 -> 3.19
[1:03:20] Using charge balance adjust
[1:03:20] Dispensed 0.002752 mL of Base (0.5 M KOH)
[1:03:40] Stirrer speed set to 0
[1:03:50] Datapoint id 55 collected
[1:03:50] Charge balance equation is out by 19.2%
[1:03:50] Stirrer speed set to 60
[1:03:55] pH 3.23 -> 3.43
[1:03:55] Using cautious pH adjust
[1:03:55] Dispensed 0.000847 mL of Base (0.5 M KOH)
[1:04:01] Stepping pH = 3.33
[1:04:01] Dispensed 0.000541 mL of Base (0.5 M KOH)
[1:04:06] Stepping pH = 3.41
[1:04:06] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:04:11] Stepping pH = 3.42
[1:04:11] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:04:16] Stepping pH = 3.43
[1:04:31] Stirrer speed set to 0
[1:04:41] Datapoint id 56 collected
[1:04:41] Charge balance equation is out by 1.6%
[1:04:41] Stirrer speed set to 60
[1:04:46] pH 3.44 -> 3.64
[1:04:46] Using charge balance adjust
[1:04:46] Dispensed 0.001105 mL of Base (0.5 M KOH)
[1:05:07] Stirrer speed set to 0

Sample name: **M02_octanol**
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Experiment start time: **3/3/2018 1:46:01 PM**
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Instrument ID: **T312060**

Experiment Log (continued)

[1:05:22] Datapoint id 57 collected
[1:05:22] Charge balance equation is out by 27.7%
[1:05:22] Stirrer speed set to 60
[1:05:27] pH 3.69 -> 3.89
[1:05:27] Using cautious pH adjust
[1:05:27] Dispensed 0.000306 mL of Base (0.5 M KOH)
[1:05:32] Stepping pH = 3.76
[1:05:32] Dispensed 0.000306 mL of Base (0.5 M KOH)
[1:05:37] Stepping pH = 3.92
[1:05:52] Stirrer speed set to 0
[1:06:03] Datapoint id 58 collected
[1:06:03] Charge balance equation is out by -0.4%
[1:06:03] Stirrer speed set to 60
[1:06:08] pH 3.93 -> 4.13
[1:06:08] Using charge balance adjust
[1:06:08] Dispensed 0.000376 mL of Base (0.5 M KOH)
[1:06:28] Stirrer speed set to 0
[1:06:39] Datapoint id 59 collected
[1:06:39] Charge balance equation is out by 41.3%
[1:06:39] Stirrer speed set to 60
[1:06:44] pH 4.23 -> 4.43
[1:06:44] Using cautious pH adjust
[1:06:44] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:06:49] Stepping pH = 4.24
[1:06:49] Dispensed 0.000259 mL of Base (0.5 M KOH)
[1:06:54] Stepping pH = 4.79
[1:07:09] Stirrer speed set to 0
[1:07:54] Datapoint id 60 collected
[1:07:54] Charge balance equation is out by -83.8%
[1:07:54] Stirrer speed set to 60
[1:08:00] pH 4.78 -> 4.98
[1:08:00] Using cautious pH adjust
[1:08:00] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:08:05] Stepping pH = 4.77
[1:08:05] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:08:10] Stepping pH = 5.22
[1:08:25] Stirrer speed set to 0
[1:08:41] Datapoint id 61 collected
[1:08:41] Charge balance equation is out by -208.6%
[1:08:41] Stirrer speed set to 60
[1:08:46] pH 5.30 -> 5.50
[1:08:46] Using cautious pH adjust
[1:08:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:08:51] Stepping pH = 5.31
[1:08:51] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:08:56] Stepping pH = 5.45
[1:08:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:01] Stepping pH = 5.56
[1:09:16] Stirrer speed set to 0
[1:10:05] Datapoint id 62 collected
[1:10:05] Charge balance equation is out by -166.1%
[1:10:05] Stirrer speed set to 60
[1:10:10] pH 5.72 -> 5.92
[1:10:10] Using cautious pH adjust
[1:10:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:15] Stepping pH = 5.75
[1:10:15] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:10:20] Stepping pH = 6.09
[1:10:35] Stirrer speed set to 0

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Experiment Log (continued)

[1:11:35] Datapoint id 63 collected
[1:11:35] Charge balance equation is out by -74.3%
[1:11:35] Stirrer speed set to 60
[1:11:41] pH 6.22 -> 6.42
[1:11:41] Using cautious pH adjust
[1:11:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:11:46] Stepping pH = 6.24
[1:11:46] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:11:51] Stepping pH = 6.31
[1:11:51] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:11:56] Stepping pH = 6.87
[1:12:11] Stirrer speed set to 0
[1:13:11] Datapoint id 64 collected
[1:13:11] Charge balance equation is out by -176.8%
[1:13:11] Stirrer speed set to 60
[1:13:16] pH 7.12 -> 7.32
[1:13:16] Using cautious pH adjust
[1:13:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:21] Stepping pH = 7.20
[1:13:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:27] Stepping pH = 7.33
[1:13:42] Stirrer speed set to 0
[1:14:42] Datapoint id 65 collected
[1:14:42] Charge balance equation is out by -102.3%
[1:14:42] Stirrer speed set to 60
[1:14:47] pH 7.16 -> 7.36
[1:14:47] Using cautious pH adjust
[1:14:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:14:52] Stepping pH = 7.24
[1:14:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:14:57] Stepping pH = 7.41
[1:15:12] Stirrer speed set to 0
[1:16:12] Datapoint id 66 collected
[1:16:12] Charge balance equation is out by -115.3%
[1:16:12] Stirrer speed set to 60
[1:16:17] pH 7.58 -> 7.78
[1:16:17] Using cautious pH adjust
[1:16:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:16:22] Stepping pH = 7.73
[1:16:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:16:28] Stepping pH = 7.93
[1:16:43] Stirrer speed set to 0
[1:17:43] Datapoint id 67 collected
[1:17:43] Charge balance equation is out by -302.3%
[1:17:43] Stirrer speed set to 60
[1:17:48] pH 7.75 -> 7.95
[1:17:48] Using cautious pH adjust
[1:17:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:17:53] Stepping pH = 7.87
[1:17:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:17:58] Stepping pH = 8.15
[1:18:13] Stirrer speed set to 0
[1:19:13] Datapoint id 68 collected
[1:19:13] Charge balance equation is out by -373.8%
[1:19:13] Stirrer speed set to 60
[1:19:18] pH 8.24 -> 8.44
[1:19:18] Using cautious pH adjust
[1:19:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:23] Stepping pH = 8.26



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Experiment start time: **3/3/2018 1:46:01 PM**
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Experiment Log (continued)

[1:19:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:28] Stepping pH = 8.42
[1:19:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:34] Stepping pH = 8.58
[1:19:49] Stirrer speed set to 0
[1:20:49] Datapoint id 69 collected
[1:20:49] Charge balance equation is out by -452.3%
[1:20:49] Stirrer speed set to 60
[1:20:54] pH 8.61 -> 8.81
[1:20:54] Using cautious pH adjust
[1:20:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:20:59] Stepping pH = 8.61
[1:20:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:21:04] Stepping pH = 8.60
[1:21:04] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:21:09] Stepping pH = 9.23
[1:21:24] Stirrer speed set to 0
[1:21:39] Datapoint id 70 collected
[1:21:39] Charge balance equation is out by -904.7%
[1:21:39] Argon flow rate set to 0
[1:21:43] Titrator arm moved over Titration position